工学系研究科専攻間横断型教育プログラム
「機械システム・イノベーション」

GMSI

最先端融合科学イノベーション
教育研究コンソーシアム

CIAiS

東京大学
THE UNIVERSITY OF TOKYO

第222回GMSI公開セミナー／第46回CIAiSセミナー

Modelling the growth of Single Walled Carbon Nanotubes

Dr. Christophe Bichara

CINaM, Aix-Marseille University and CNRS

日 時: 2017年3月7日(火) 14:00－15:30
場 所: 東京大学工学部2号館 3F 31A会議室

Since 25 years, significant progress has been achieved in the controlled synthesis of Single Walled Carbon Nanotubes (SWNTs), but we are still facing difficult issues concerning the yield and selectivity of their synthesis by Chemical Vapor Deposition. In such a complex problem, real understanding only results from coupling different experimental techniques, from chemical engineering approaches to atomic scale investigations by e.g. Transmission Electron Microscopy, with modelling and computer simulations.
In this context, we developed an original atomistic metal-carbon interaction model, based on a tight binding approximation, coupled with Monte Carlo simulations in canonical and Grand Canonical ensembles[1]. In close collaboration with experimental groups, supported by different projects among which the Japan / EU project IRENA, we analyzed different aspects of SWNT growth and present some of them here.
We first focus on a simple catalyst (Ni) and investigate tube nucleation[2] and the state of the catalyst in presence of carbon[3]. Sustainable tube synthesis requires a dewetting of the catalyst nanoparticle, along with the growth of the carbon walls, to avoid its encapsulation and deactivation. We show that the properties of the Ni/sp^2 carbon interfaces are driven by the carbon fraction dissolved in the NP[4] that depends on the CVD process parameters, in particular on the choice of the carbon bearing precursor. These different carbon feeding regimes give rise to different growth modes[5], corresponding to different structures of the NP/nanotube contact areas. For carbon saturated nanoparticles[7], the interface is reduced to a line contact, in which case a near armchair selectivity is sometimes reported, while lower dissolved carbon fractions lead to a lateral surface contact between the tube and the catalyst NP[8]. Both situations will be discussed in terms of yield and selectivity, in close connection with experimental results.

References

[1] Amara, H. *et al.* Phys. Rev. B **79**, 014109 (2009).
[2] Amara, H. *et al.* Phys. Lett. **100**, 056105 (2008).
[3] Magnin, Y. *et al.* Phys. Rev. Lett., **115**, 205502, (2015).
[4] Diarra, M. *et al.* Phys. Rev. Lett., **109**, 185501 (2012).
[5] Fiawoo, M.-F. C. *et al.* Phys. Rev. Lett., **108**, 195503 (2012).
[6] Weatherup, R. S. *et al.* J. Am. Chem. Soc., **136**, 13698–13708 (2014).
[7] He, M. *et al.* Carbon, **113**, 231-6 (2017) ; Nanoscale **4**, 7394 (2012).
[8] J .-M. Aguiar-Hualde *et al.* “Probing the role of carbon solubility in transition metal catalyzing Single-Walled Carbon Nanotubes growth” submitted.

主催: 東京大学大学院工学系研究科「機械システム・イノベーション」プログラム（GMSI）
「最先端融合科学イノベーション教育研究コンソーシアム」（CIAiS）
本件連絡先: 東京大学大学院工学系研究科機械工学専攻 教授 丸山 茂夫
GMSIプログラム事務局 E-mail: office@gmsi.t.u-tokyo.ac.jp Phone: 03-5841-0696